



Consistency tests in guaranteed simulation of nonlinear uncertain systems with application to an activated sludge process

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Abstract

In this paper, interval arithmetic simulation techniques are presented to determine guaranteed enclosures of the state variables of both continuous and discrete-time systems with uncertain but bounded parameters. In nonlinear uncertain systems axis-parallel interval boxes are mapped to complexly shaped regions in the state space that represent sets of possible combinations of state variables. The approximation of each region by a single interval box causes an accumulating overestimation from time-step to time-step, usually called the wrapping effect. The algorithm presented in this paper minimizes the wrapping effect by applying consistency techniques based on interval Newton methods. Subintervals that do not belong to the exact solution at a given time can be eliminated in order to give a tighter but still conservative approximation of the exact solution. Additionally, efficient splitting and merging strategies are employed to limit the number of subintervals. The proposed algorithm is applied to the simulation of an activated sludge process in biological wastewater treatment.

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1. Introduction

The simulation of nonlinear systems with uncertain system parameters is a common problem in various disciplines of engineering. Popular approaches to simulate uncertain systems are Monte Carlo methods. However, these methods are not suitable if guaranteed bounds of the state variables are required, which is important for security relevant system operation. In real-world applications mostly only lower and upper bounds of the uncertain parameters are known. Consequently, application of interval methods [2] to the evaluation of mathematical system models leads to conservative estimations of the lower and upper bounds of the state variables. However, a naive application of interval methods results in huge overestimation. Using only one axis-parallel interval box it is impossible to represent complexly shaped regions of state variables in the state space. The replacement of these regions by axis-parallel enclosures in each time-step leads to accumulation of overestimation over simulation time, also known as the wrapping effect. This kind of overestimation is reduced by removing subintervals of an axis-parallel box that do not belong to the exact solution of the state equation with respect to the approximation of the previous time step. This is done by the consistency techniques described in this paper. In addition the time-discretization of the continuous-time system leads to a truncation error. It

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is shown how the truncation error can be included in the consistency test. In Section 2, the formulation of the problem is given. In Section 3, the proposed simulation algorithm based on consistency techniques is described. In Section 4, simulation results of a subprocess for biological wastewater treatment are shown. Section 5 describes how the truncation error can be calculated and included in the consistency test. Finally, conclusions and an outlook on future research are given in Section 6.

2. Problem formulation

A nonlinear uncertain system can be described by the following differential equation:

$$\dot{x}(t) = f(x(t), p(t)) \quad (1)$$

with the state vector x and the uncertain parameter vector p . For simulation purposes the continuous system has to be discretized in time. This is done by Taylor series expansion

$$x(t_k + T) = x(t_k) + T f^{(0)}(t_k, x(t_k), p_k) + \frac{T^2}{2!} f^{(1)}(t_k, x(t_k), p_k) + \dots + \frac{T^\tau}{\tau!} f^{(\tau-1)}(t_k, x(t_k), p_k) + e(\xi, x(\xi), p_k) \quad \text{with } t_k < \xi < t_k + T \quad (2)$$

with the integration step-size T , i.e., $t_k = kT$ and $t_k < \xi < t_{k+1}$. Throughout this paper, all uncertain system parameters $p_k \in [\underline{p}_k, \overline{p}_k]$ are assumed to be interval parameters, i.e., the range of these parameters is defined by lower bounds \underline{p}_k and upper bounds \overline{p}_k . The parameters are assumed to be time-varying, i.e., arbitrary variations of the actual value of these parameters from one time-step to the next are allowed within the specified parameter range without specifying any dynamical behavior of the parameter variation. First, the truncation error is neglected and the Taylor series is truncated after $\tau = 1$ which gives

$$x_{k+1} = x_k + T f(x_k, p_k). \quad (3)$$

This corresponds to the explicit Euler method and f corresponds to $f^{(0)}$. If the system Eq. (3) is evaluated for a given interval box $[x_k^T, p_k^T]^T$ in a naive way, a single interval box is obtained, even though the actual solution may be complexly shaped. If this is repeated from time-step to time-step huge overestimation may occur. This overestimation—also known as the wrapping effect—is reduced by applying consistency techniques presented in Section 3. By this procedure, the influence of parts of the state space without physical relevance to the considered activated sludge process is minimized.

3. Consistency techniques

In this section a simulation algorithm based on consistency techniques is described. The algorithm consists of two steps: A forward step which calculates rough conservative enclosures of the state variables in the following time-step and a backward step, which deletes subintervals which do not belong to the exact solution with respect to the previous approximation [1].

3.1. Forward step

In the forward step the system Eq. (3) is evaluated with a monotonicity test and iterative calculation of infimum and supremum. These methods are described in [4].

3.2. Backward step

During backward computation of a subinterval SI three different cases have to be distinguished. These three cases are illustrated in Fig. 1. Applying the backward step, subinterval $SI1$ in time-step $k + 1$ is mapped to $SI1'$ in time-step k . $SI1'$ lies completely out of x_k , therefore $SI1$ does not belong to the exact solution. Subinterval $SI2'$ lies completely

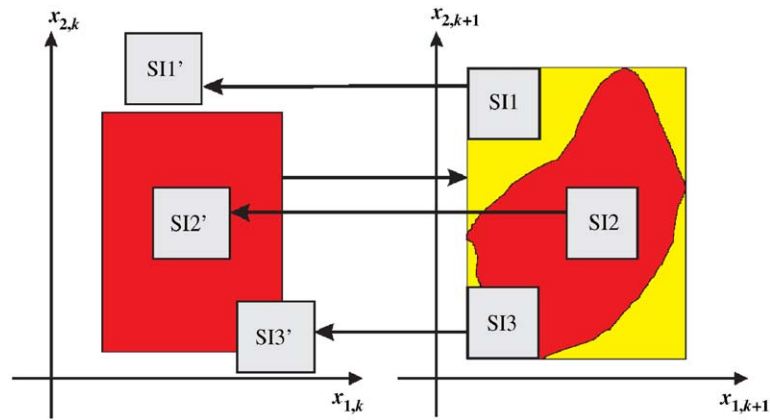


Fig. 1. Forward step and backward step.

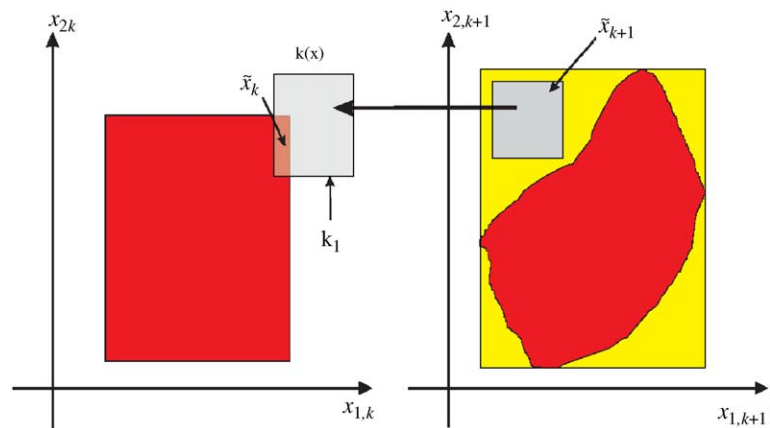


Fig. 2. Determination of splitting direction.

inside of x_k . That means $SI2$ belongs to the exact solution of time-step $k + 1$. Subinterval $SI3$ has to be split further, because $SI3'$ is only included partially in x_k and therefore no conclusion can be made. The repeated application of splitting and backward calculation improves the approximation of the actual solution in time-step $k + 1$. The backward step is derived from Eq. (3) by rewriting it the following way:

$$0 = x_k + Tf(x_k, p_k) - x_{k+1} = h(x_k, p_k). \quad (4)$$

Next, x_{k+1} is split into several subintervals \tilde{x}_{k+1} . Now it has to be tested if there exists a region of zeros in x_k for every \tilde{x}_{k+1} . If there exists a region of zeros in x_k , then \tilde{x}_{k+1} belongs to x_{k+1} . If not, \tilde{x}_{k+1} is deleted. If no conclusion can be made, \tilde{x}_{k+1} has to be split again. Eq. (4) is solved by applying the Krawczyk method [3]. The advantage of the Krawczyk method over other interval Newton approaches is that inversion of interval matrices is avoided. The result of the Krawczyk iteration rule is denoted by $k(x)$ and will be needed in the next subsection.

3.3. Splitting strategy

To keep the number of splitting operations and subintervals as low as possible, efficient splitting strategies are required. In most cases a cyclical change of the splitting direction is inefficient. In this paper an heuristic splitting strategy is applied to remove inconsistent subintervals as soon as possible, see Fig. 2. If $k(x)$ is the result of the backward step,

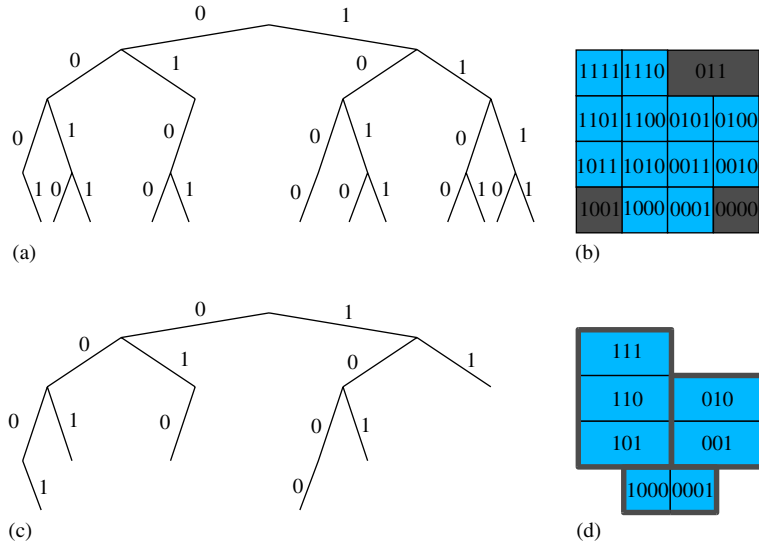


Fig. 3. Merging routine: (a) tree after splitting and deleting of inconsistent subintervals; (b) intervals after splitting and deleting of inconsistent subintervals; (c) tree after merging; and (d) intervals after merging.

first the component k_l , with least intersection of $k(x)$ with x_k is determined. This is done by the following expression

$$\min_{i=1 \dots \text{length}(x_k)} \left\{ \frac{\text{diam}(\tilde{x}_{i,k})}{\text{diam}(k_i)} \right\} \Rightarrow l, \quad (5)$$

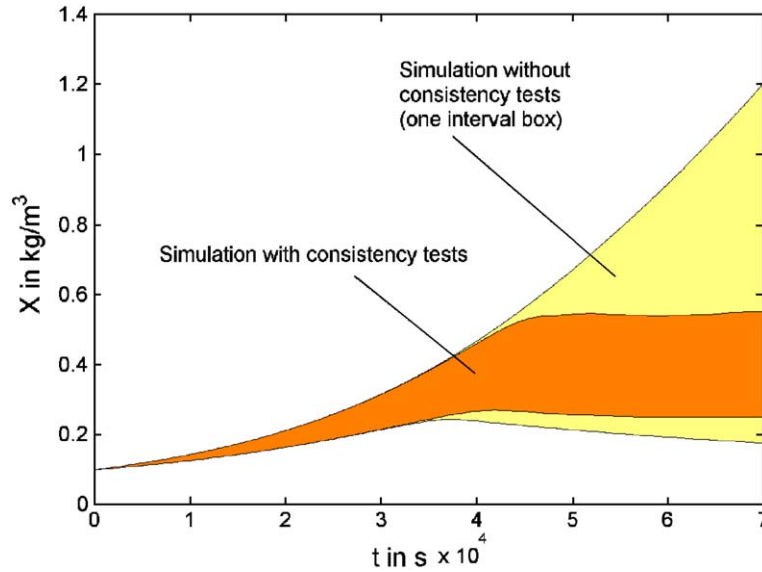
where \tilde{x}_k is the intersection of x_k and $k(x)$ and $\text{diam}(\tilde{x}_{i,k})$ the diameter of $\tilde{x}_{i,k}$. Next, the component $\tilde{x}_{j,k+1}$ of \tilde{x}_{k+1} with the biggest influence on k_l is determined with

$$\max_{i=1 \dots \text{length}(x_k)} \left\{ \left| \frac{\partial k_l}{\partial \tilde{x}_{i,k+1}} \text{diam}(\tilde{x}_{i,k+1}) \right| \right\} \Rightarrow j. \quad (6)$$

Finally, \tilde{x}_{k+1} is split at the midpoint of the component j .

3.4. Merging strategy

The consistency test and the associated splitting leads inevitably to an increasing number of intervals. To avoid an exponential growth of the interval number from time-step to time-step also efficient merging strategies have to be applied. Two intervals can be merged if the smallest interval around both leads to no or only little overestimation. The merging consists of several steps. During the splitting of an interval each subinterval gets a binary number which is stored in a tree structure. If an interval is split into two subintervals each subinterval gets a new binary number consisting of the binary number of the original interval and an additional 0 or 1, respectively, at the end leading to a binary tree with two new branches after each splitting. If an interval is deleted by the consistency test no new branches arise from this interval. After the splitting the tree gives information about intervals which can be merged without further overestimation. It just has to be checked if two subintervals descend from the same original interval. This is the case if the corresponding binary number differs only at the last digit. After the merging with the help of the tree there may be still some intervals left which could be merged. Therefore a second routine is applied. This routine calculates the sum of the pseudo volume of two intervals and the volume of the smallest interval around both. If this volume is not or only a little bit larger than the sum of the volumes of the original intervals, the corresponding intervals are merged. The merging routine is illustrated in Fig. 3. The dark gray intervals (Fig. 3(b)) have been deleted exemplarily as well as the corresponding branches in binary tree (Fig. 3(a)). The gray boxes around the intervals in Fig. 3(d) mark intervals which are merged by the second merging routine.

Fig. 4. Bacteria concentration X .

4. Simulation results

In this section, the proposed interval arithmetic simulation algorithm is applied to a simplified Activated Sludge Model (ASM) in biological wastewater treatment which is described by the following set of differential equations:

$$\begin{aligned}
 \dot{S} &= \frac{Q_W}{V_A}(S_W - S) - \mu(S, S_O) \frac{1}{Y} X, \\
 \dot{X} &= -\frac{Q_W}{V_A} X + \frac{Q_{RS}}{V_A}(X_{Set} - X) + (\mu(S, S_O) - b) X, \\
 \dot{S}_O &= \frac{Q_W}{V_A}(S_{OW} - S_O) - \mu(S, S_O) \frac{1-Y}{Y} X + \frac{\rho_{O_2}}{V_A} \left(1 - \frac{S_O}{S_{O,sat}}\right) u_{O_2}, \\
 \dot{X}_{Set} &= \frac{(Q_W + Q_{RS})X - (Q_{EX} + Q_{RS})X_{Set}}{V_{Set}}
 \end{aligned} \tag{7}$$

with

$$\mu(S, S_O) = \hat{\mu}_H \frac{S}{S + K_S} \frac{S_O}{S_O + K_{OS}}. \tag{8}$$

The four state variables represent the concentration S of biologically degradable organic matter (substrate), the concentration X of substrate consuming bacteria, the concentration S_O of dissolved oxygen in the aeration tank, and the concentration X_{Set} of bacteria in the settler. For the state variables the following restrictions must hold additionally:

$$S \geq 0, \quad X \geq 0, \quad X_{Set} \geq 0, \quad 0 \leq S_O \leq S_{O,sat}. \tag{9}$$

These inequalities point out the physical restrictions, namely, all concentrations have to be non-negative for all times. Furthermore, the concentration S_O of dissolved oxygen is limited by the saturation concentration $S_{O,sat}$. The nominal values of the system parameters are given in [4]. The uncertainty of the maximum specific growth rate $\hat{\mu}_H$ of the heterotrophic biomass is known to be $\hat{\mu}_H \in [0.9; 1.1]\mu_{H,nominal}$. Fig. 4 shows a comparison between the simulation results with consistency tests and without consistency tests for the bacteria concentration X in the aeration tank. In the simulation without consistency test only one subinterval was used and only the forward step was applied. A fixed

step-size $T = 40s$ has been used. The maximum number of intervals in the simulation with consistency test is 500. The consistency test is applied to the 20 largest intervals, which is a sensible compromise between simulation quality and computing time. Those 20 intervals are split first and the consistency test is applied to the now 40 subintervals. Subintervals which can be excluded are deleted from the list, intervals which belong to the solution are inserted into another list. The remaining intervals are split again. This procedure is repeated until a maximum of 5000 intervals is reached. At the end of each time-step a merging routine is applied. If there are still more than 500 intervals left after the merging routine only the forward step is applied until the merging routine at the end of each time-step reduces the number to less than 500. The simulation results make clear that a simulation with only one interval box leads to much too conservative results. The application of consistency tests gives much tighter results which do not explode to meaningless width.

5. Time-discretization error

In this section it is shown how to include the truncation error in the consistency test in order to get also guaranteed bounds of the continuous-time system. Consider the Taylor series expansion in Eq. (2). For the truncation error $e(\xi, x(\xi), p_k)$ guaranteed bounds are obtained with

$$e(\xi, x(\xi), p_k) \subseteq \frac{T^{\tau+1}}{(\tau+1)!} f^{(\tau)}([t_k; t_k + T], B, p_k). \quad (10)$$

In this expression, the interval B is a bounding box for the range of the state variables $x(t) \in B \forall t \in [t_k; t_{k+1}]$, if the initial intervals $x_k = x(t_k)$ are given. Applying the Picard Operator

$$\Phi(B) = x(t_k) + [0; T]f([t_k; t_{k+1}], B, p_k) \quad (11)$$

the interval enclosure B can be determined [1]. B is a bounding box if $\Phi(B) \subseteq B$. For the explicit Euler method including the truncation error

$$x(t_k + T) \subseteq x(t_k) + Tf^{(0)}(t_k, x(t_k), p_k) + e([t_k; t_k + T], B, p_k) \quad (12)$$

is obtained. The interval box $x(t_k + T)$ is a guaranteed bound of all state variables at $t_k + T$. For the consistency test this equation has to be rewritten according to

$$0 = x_k + Tf(x_k, p_k) + e(x_k, p_k) - x_{k+1} = h(x_k, p_k). \quad (13)$$

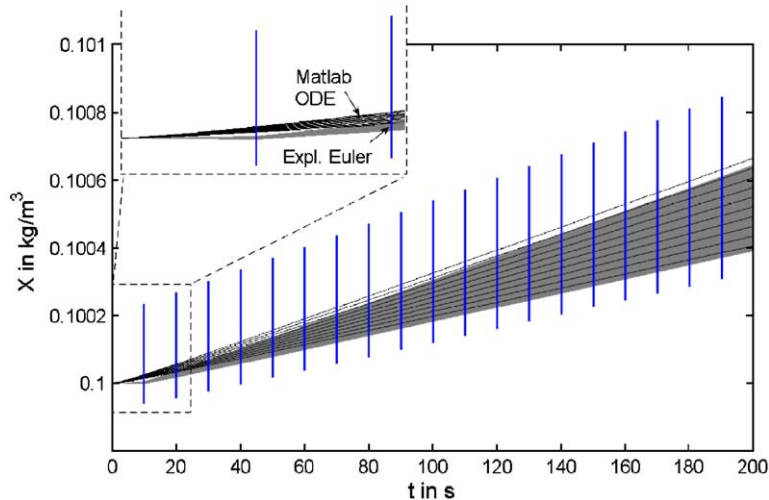


Fig. 5. Influence of the truncation error.

The following steps of the algorithm are the same as before. The influence of the truncation error on the simulation results is shown in Fig. 5 for the bacteria concentration X . The thin trajectories are solutions of the Matlab ODE-solver with very low tolerances for 10 different values of the maximum specific growth rate. The gray curve shows the solution of the interval simulation without consideration of the truncation error. It can be seen that the solutions of the Matlab ODE solver are not always included. The vertical lines mark the results of an interval simulation at the sampling points with truncation error. Now the solutions of the Matlab ODE solver are included.

6. Conclusions

In this paper, an interval arithmetic simulation approach for systems with uncertain parameters has been proposed. The application to an activated sludge model of biological wastewater treatment has pointed out that the proposed consistency tests reduce the wrapping effect significantly compared to huge overestimation occurring in simulations with only one interval box. Further improvement of the splitting and merging strategies, will increase the simulation quality. Additionally, the forward step can be optimized by applying a recursive pseudo-linear state transformation [4] or an implicit integration method.

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